

# Structural Tuning of Two-Dimensional Perovskites at High Pressure

Lauren DiLoreto

Department of Chemistry, University of Western Ontario



Western

## Introduction

- Characterize 2D-Perovskites:  $\text{DPDAPbI}_4$  and  $\text{CMApPbI}_4$  at high pressure
- Many opto-electronic applications such as solar cells
- Objective is to observe irreversible changes to optimize efficiency in its application

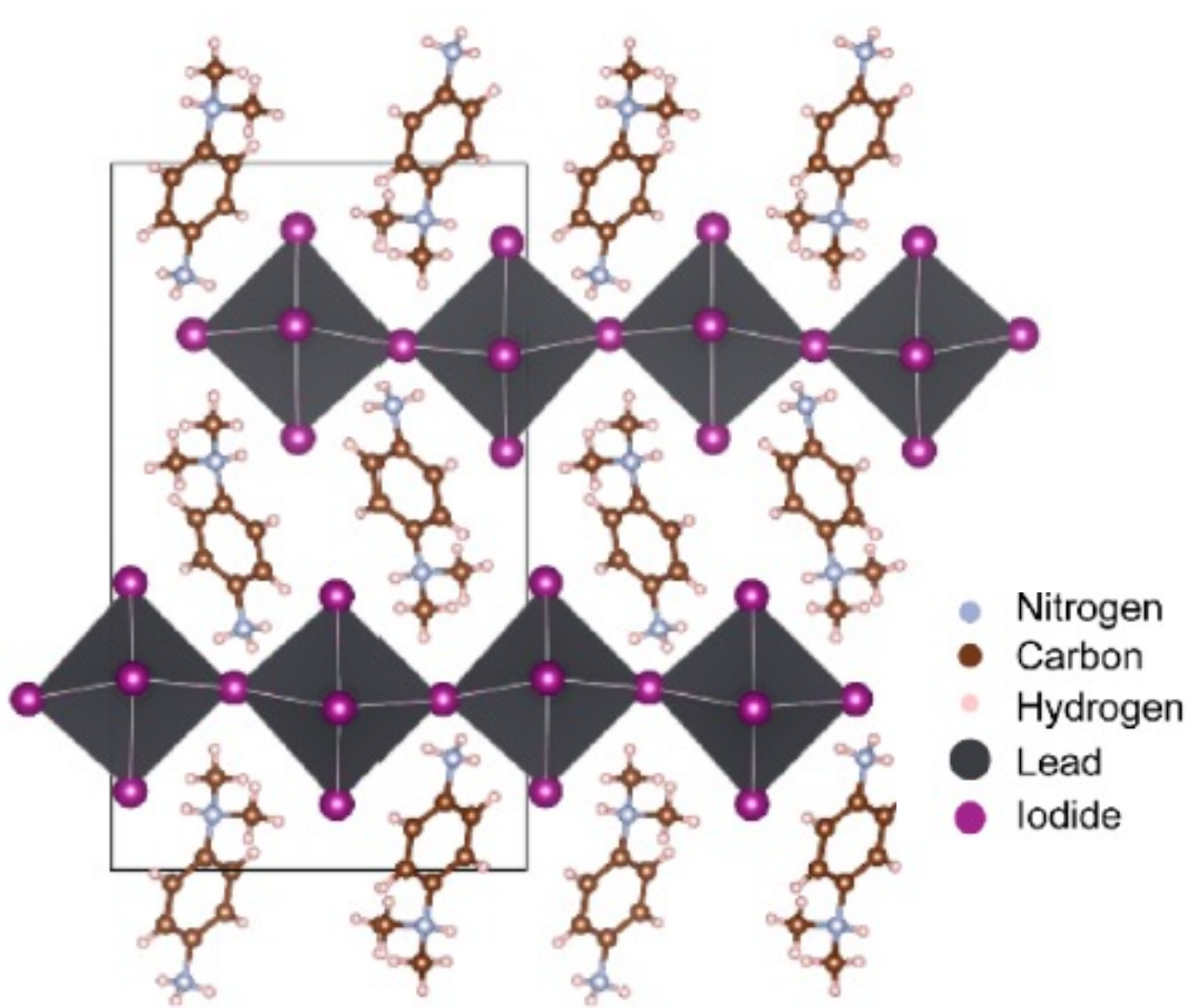


Illustration of  $\text{DPDAPbI}_4$  crystal structure

$\text{CMA}_2\text{PbI}_4$  lattice structure similar to that of  $\text{DPDAPbI}_4$  with CMA as the organic spacer

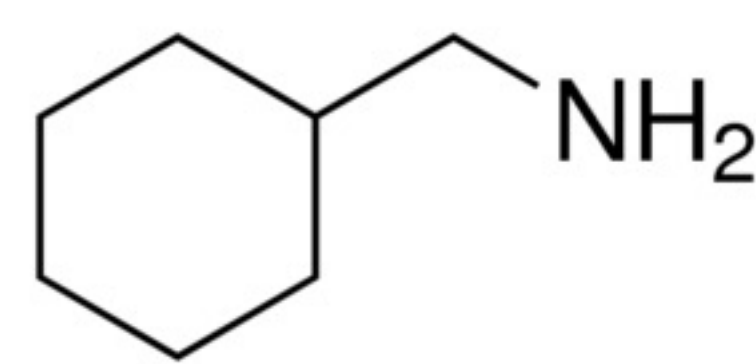
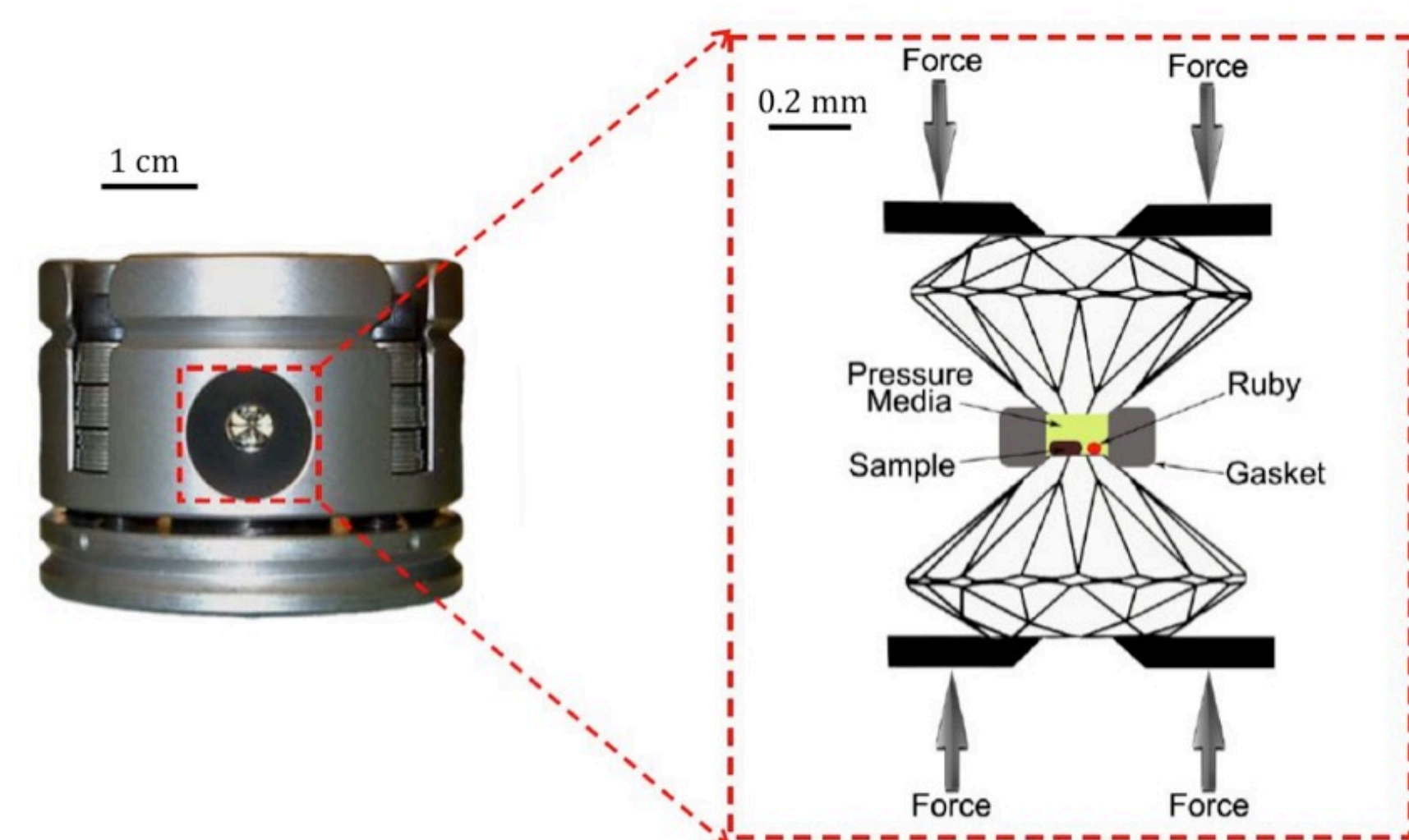


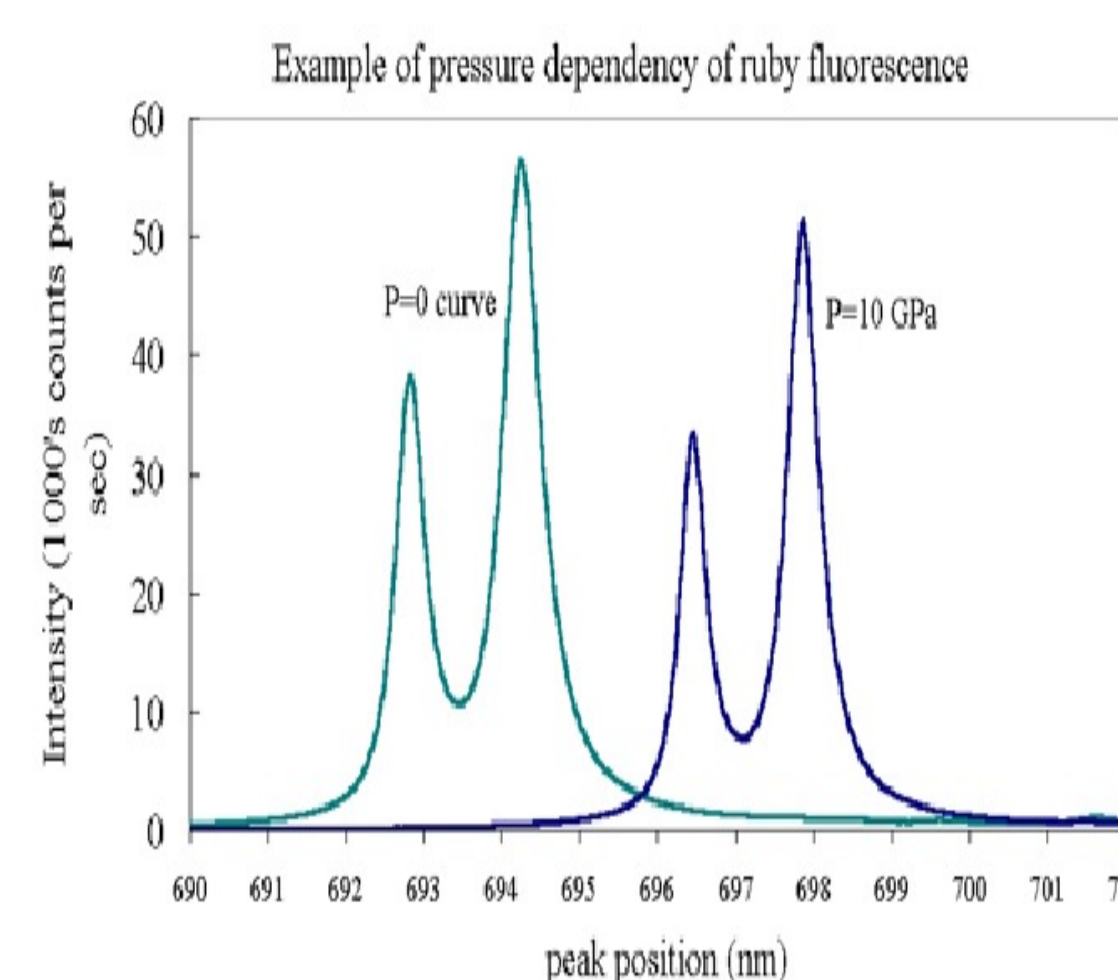
Photo of Cyclohexane Methyl Amine (CMA)

## Experimental



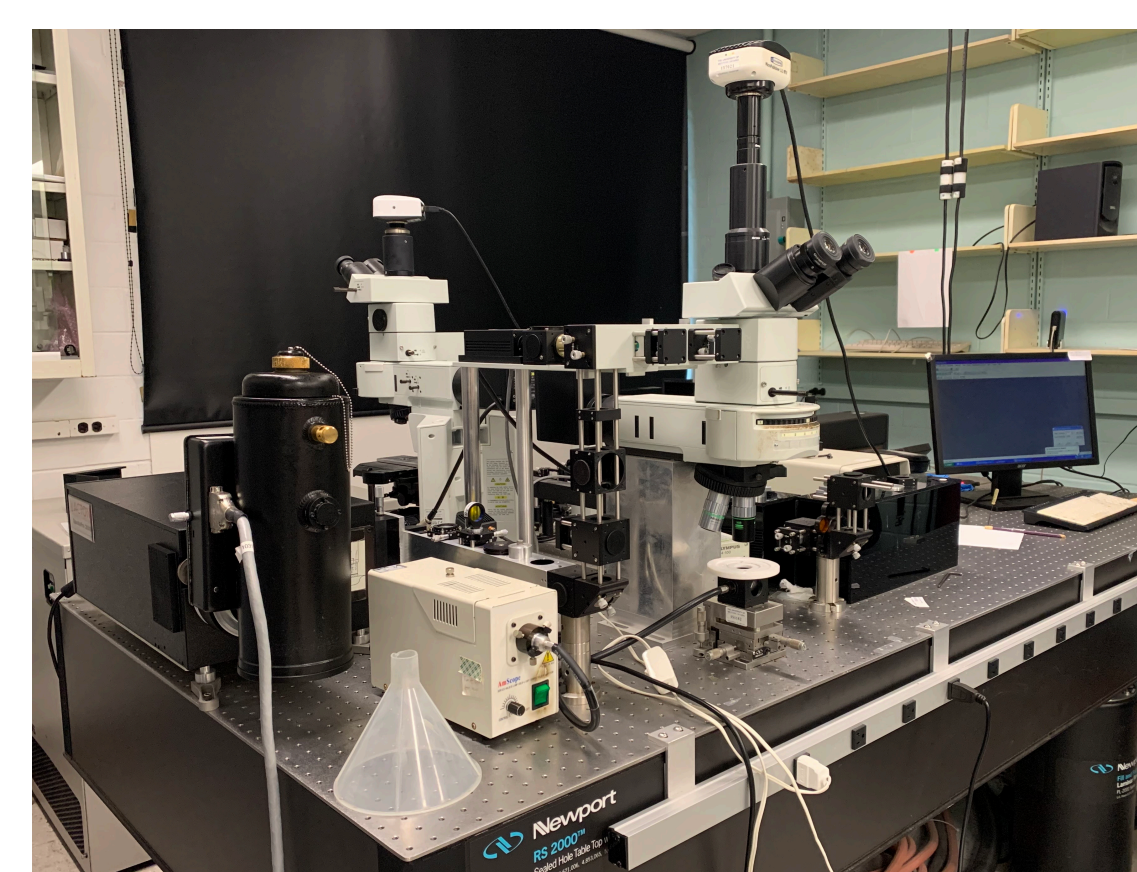
Diamond Anvil Cell (DAC)

- Used to apply static pressure to the sample



Ruby fluorescence

- Used to determine the pressure of the sample inside of DAC



Raman Spectroscopy

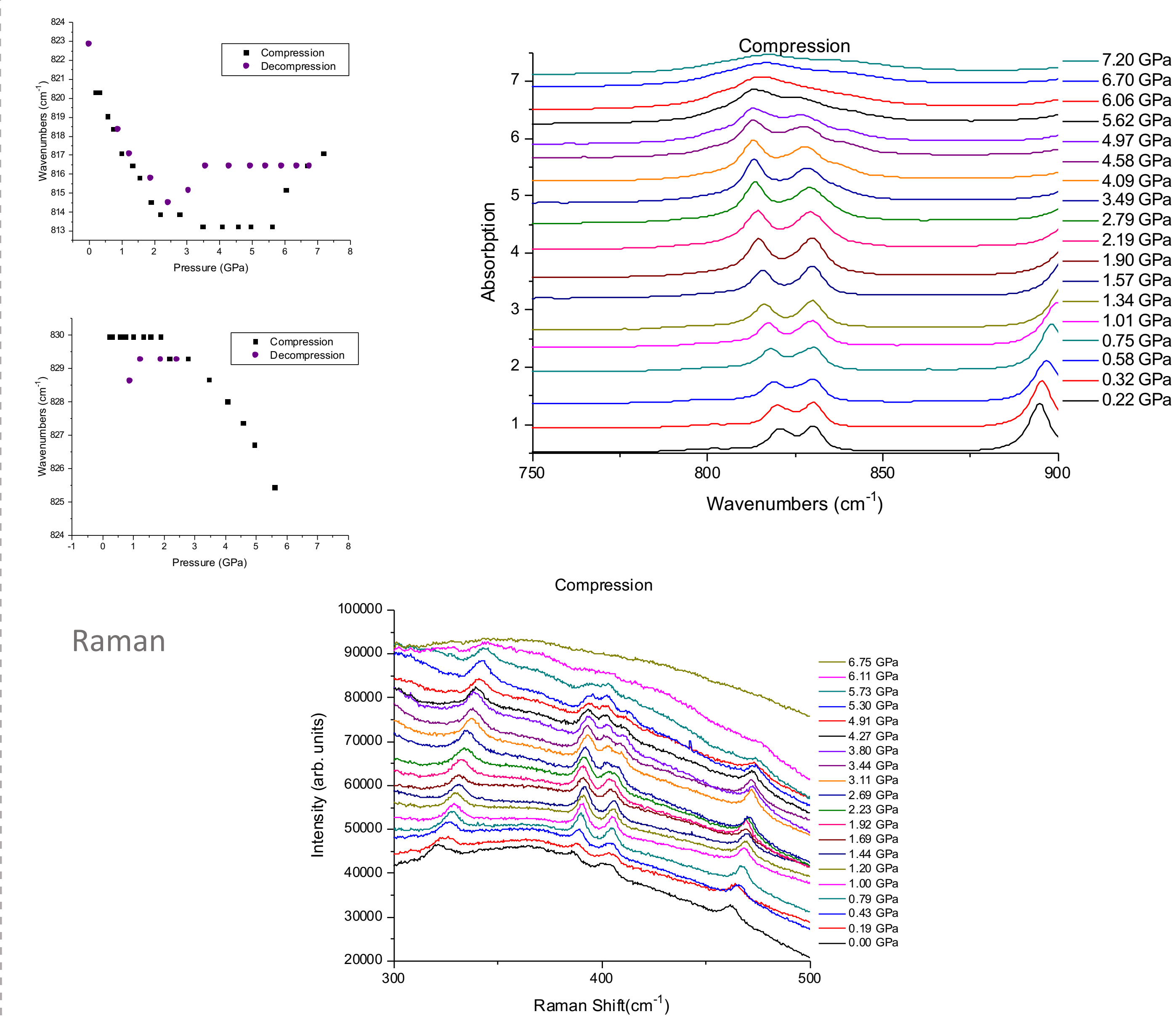
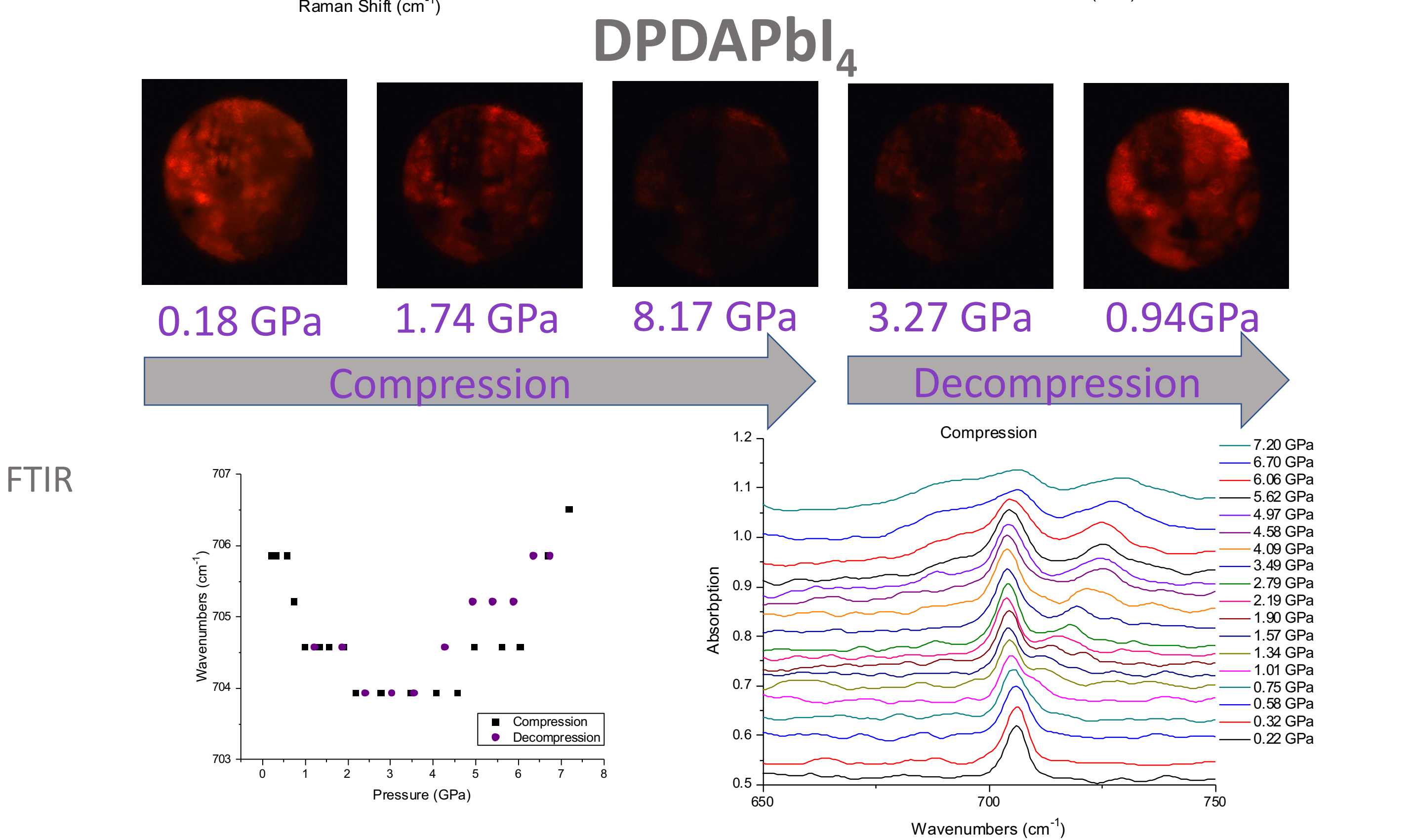
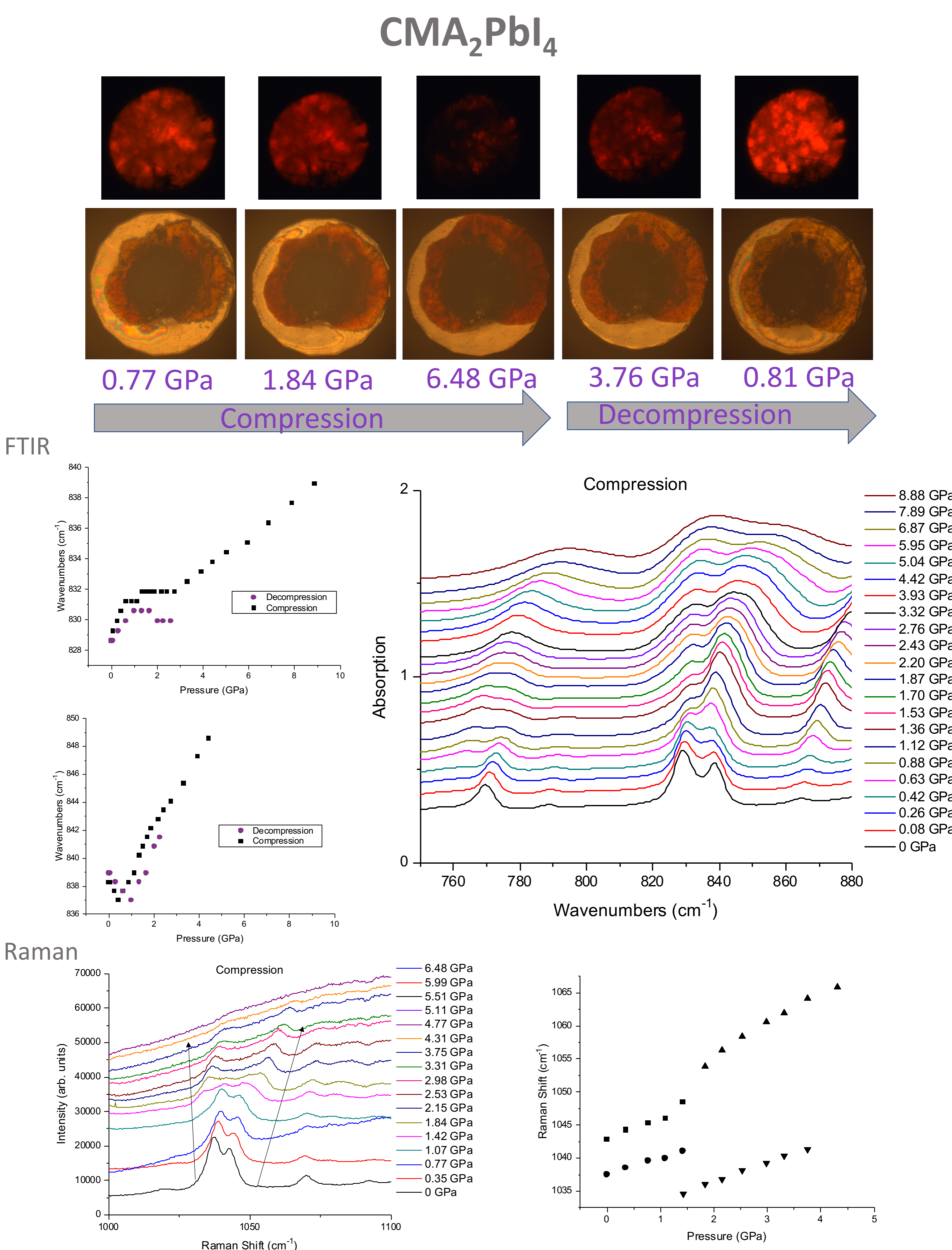
- Measures vibrational frequencies based on the inelastic scattering of light from the sample



Fourier-Transform Infrared Spectroscopy (FTIR)

- Measures the frequencies at which a sample absorbs IR radiation corresponding to vibrations

## Results



## Conclusions

- Both materials underwent a reversible amorphization
- Metastable change did not occur
- Potential phase change at  $\sim 2$  GPa and  $\sim 5$  GPa for  $\text{DPDAPbI}_4$  and at  $\sim 0.5$  GPa,  $\sim 1.5$  GPa, and  $\sim 3$  GPa for  $\text{CMA}_2\text{PbI}_4$
- Further research to determine band gap energy, photoluminescent properties, and confirm suspected phase changes

## References

- Birkner, N. How an FTIR Spectrometer Operates. [https://chem.libretexts.org/Bookshelves/Physical\\_and\\_Theoretical\\_Chemistry\\_Textbook\\_Maps/Supplemental\\_Modules\\_\(Physical\\_and\\_Theoretical\\_Chemistry\)/Spectroscopy/Vibrational\\_Spectroscopy/Infrared\\_Spectroscopy/How\\_an\\_FTIR\\_Spectrometer\\_Operates](https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Spectroscopy/Vibrational_Spectroscopy/Infrared_Spectroscopy/How_an_FTIR_Spectrometer_Operates) (accessed Aug 14, 2021).
- Dong, Z.; Song, Y. Novel Pressure-Induced Structural Transformations of Inorganic Nanowires. *Nanowires - Fundamental Research* **2011**.
- Guide to Raman spectroscopy. <https://www.bruker.com/en/products-and-solutions/infrared-and-raman/raman-spectrometers/what-is-raman-spectroscopy.html> (accessed Aug 14, 2021).
- Matthew P. Hautzinger, Jun Dai, Yujin Ji, Yongping Fu, Jie Chen, Ilia A. Guzei, John C. Wright, Youyong Li, and Song Jin *Inorganic Chemistry* **2017** 56 (24), 14991-14998
- Ruby Fluorescence; 2018.
- Wei, Y.; Chu, H.; Tian, Y.; Chen, B.; Wu, K.; Wang, J.; Yang, X.; Cai, B.; Zhang, Y.; Zhao, J. Reverse-Graded 2D Ruddlesden-Popper Perovskites for Efficient Air-Stable Solar Cells. *Advanced Energy Materials* **2019**, 9 (21), 1900612

## Acknowledgements

- Funding: UWO, USRI, NSERC
- Supervision: Jesse Ratte, Prof. Song